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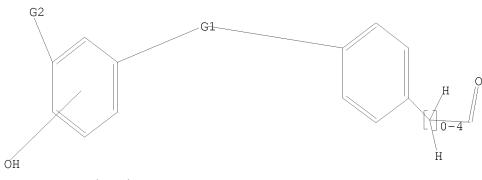
L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

L1 STR



G1 O, S, Se, CH2, SO2, NH

G2 O, Cy

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 15:57:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1421473 TO ITERATE

70.3% PROCESSED 1000000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.11

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164 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1421473 TO 1421473
PROJECTED ANSWERS: 188 TO 278

L2 164 SEA SSS FUL L1

L3 41 L2

=> s 13 and py<2003 22929827 PY<2003 L4 21 L3 AND PY<2003

=> d 1-21 ibib abs hitstr

L4 ANSWER 1 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:675334 CAPLUS

DOCUMENT NUMBER: 138:4461

AUTHOR(S):

TITLE: Synthesis of 3-(3,4-dihydroxyphenyl)-propionic acid

> derivatives by N-coupling of amines using laccase Mikolasch, Annett; Hammer, Elke; Jonas, Ulrike;

Popowski, Katrin; Stielow, Anne; Schauer, Frieder CORPORATE SOURCE: Institut fur Mikrobiologie, Ernst-Moritz-Arndt-

Universitat Greifswald, Greifswald, D-17489, Germany

SOURCE: Tetrahedron (2002), 58(38), 7589-7593

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:4461

Derivatization of the natural compound 3-(3,4-dihydroxyphenyl)-propionic acid (dihydrocaffeic acid) can be achieved by laccase-catalyzed N-coupling of aromatic and aliphatic amines. Incubation of 3-(3,4-dihydroxyphenyl)propionic acid and 4-aminobenzoic acid with laccase in aqueous medium and in the presence of oxygen yielded 3-[6-(4-carboxyphenyl)amino-3,4dihydroxyphenyl]-propionic acid as the main product (>80%). Reaction with

hexylamine resulted in 3-(6-hexylamino-3,4-dihydroxyphenyl)-propionic acid as the only product (60%).

476614-58-1P ΙT

> RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(laccase-catalyzed N-coupling of aromatic and aliphatic amines in preparation of

3-(3,4-dihydroxyphenyl)-propionic acid derivs.)

RN 476614-58-1 CAPLUS

Benzenepropanoic acid, 2-[(4-carboxyphenyl)amino]-4,5-dihydroxy- (CA CN INDEX NAME)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

2002:633267 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 137:325735

TITLE: Synthesis and characterization of hyperbranched

polybenzoxazoles

Hong, Chi-Sun; Jikei, Mitsutoshi; Kakimoto, Masa-Aki AUTHOR(S): CORPORATE SOURCE: Department of Organic and Polymeric Materials, Tokyo

Institute of Technology, Tokyo, 152-8550, Japan

SOURCE: Journal of Photopolymer Science and Technology (

2002), 15(2), 219-222

CODEN: JSTEEW; ISSN: 0914-9244

PUBLISHER: Technical Association of Photopolymers, Japan

DOCUMENT TYPE: Journal LANGUAGE: English

AB Polymerization of 3,5-bis(4-carboxyphenoxy)-2-aminophenol hydrochloride in NMP

in

the presence of Et3N, di-Ph (2,3-dihydro-2-thioxo-3-benzoxazolyl)phosphonate, and 2-amino-4-tert-butylphenol end-capping agent gave a soluble poly(o-hydroxyamide) which was cyclized by heat or by reaction in polyphosphoric acid at 130° for 6 h to the corresponding polybenzoxazole which exhibited good solubility in aprotic solvents and thermal stability.

IT 473702-29-3P, 3,5-Bis(4-carboxyphenoxy)-2-aminophenol hydrochloride

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(monomer; synthesis and characterization of heat-resistant hyperbranched polybenzoxazoles from bis(carboxyphenoxy)aminophenol hydrochloride)

RN 473702-29-3 CAPLUS

● HCl

IT 473702-30-6DP, 3,5-Bis(4-carboxyphenoxy)-2-aminophenol
 hydrochloride homopolymer, reaction products with amino-tert-butylphenol
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(polybenzoxazole precursor; synthesis and characterization of heat-resistant hyperbranched polybenzoxazoles from bis(carboxyphenoxy)aminophenol hydrochloride)

RN 473702-30-6 CAPLUS

CN Benzoic acid, 4,4'-[(4-amino-5-hydroxy-1,3-phenylene)bis(oxy)]bis-, hydrochloride, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 473702-29-3

CMF C20 H15 N O7 . C1 H

● HCl

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:207561 CAPLUS

DOCUMENT NUMBER: 136:248400

TITLE: Soluble multibranched polyimides and manufacturing

methods therefor

INVENTOR(S): Kakimoto, Masaaki; Terazakai, Mitsutoshi; Yamanaka,

Kazuhiro

PATENT ASSIGNEE(S): Rikogaku Shinkokai, Japan SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
	JP 2002080597	A	20020319	JP 2000-269155	20000905 <			
PRIO:	RITY APPLN. INFO.:			JP 2000-269155	20000905			
AB Polyimides are prepared from (R1HN)(R2HN)Ar(CO2R3)(CO2R4), where Ar is a								
	tetravalent organic groups, R1, R2 = H or Me3Si, R1 = R2 or R1 \neq R2,							
	R3, R4 = C1-10 alkyl, aryl, or Me3Si, R3 = R4 or R3 \neq R4. Thus,							
	3,5-bis(4-aminophenoxy)diphenyl ether 3',4-dicarboxylic acid mono-							
	was prepared and po	lymeriz	ed					
ΙT	332837-59-9P	_						
	RL: IMF (Industrial	manufa	cture); RCT	(Reactant); PREP (Prepa	aration); RACT			

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(manufacture of aromatic diamine dicarboxylic acid esters for soluble multibranched polyimides)

RN 332837-59-9 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4-(3,5-dihydroxyphenoxy)- (CA INDEX NAME)

L4 ANSWER 4 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:252965 CAPLUS

DOCUMENT NUMBER: 134:281290

TITLE: Polyimides with good solubility and their manufacture INVENTOR(S): Kakimoto, Masaaki; Terazakai, Mitsutoshi; Yamanaka,

Kazuhiro

PATENT ASSIGNEE(S): Zaidan Hojin Rikogaku Shinkokai, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 40 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 2001098071	A	20010410	JP 2000-200862		20000703 <
JP 3546303	В2	20040728			
PRIORITY APPLN. INFO.:			JP 1999-210653	Α	19990726
GI					

AB The polyimides, useful for elec. insulators, etc., comprising repeating units of I, II, and III (Ar = tetravalent organic group; abN, cdN, efN = unsubstituted amino, cyclic amide, C1-10-alkyl, aryl, trimethylsilyl, C2-7-hydrocarbylene, mono- or divalent acyl-substituted amino; cdN and efN may form NHXNH; X = hydrocarbylene, acyl) are manufactured Thus, 4-[3,5-bis(4-aminophenoxy)phenoxy]-1,2-benzenedicarboxylic acid monomethyl ester was polymerized, treated with heptanoyl chloride, and heated in the presence of acetic anhydride to give a polyimide with good solubility in organic

solvents.

IT 332837-59-9P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(manufacture of polyimides with good solubility)

RN 332837-59-9 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4-(3,5-dihydroxyphenoxy)- (CA INDEX NAME)

L4 ANSWER 5 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:231090 CAPLUS

DOCUMENT NUMBER: 135:40429

TITLE: Computer-aided design of molecules possessing

antiasthmatic properties based on computer QSAR

analysis

AUTHOR(S): Shilova, E. V.

CORPORATE SOURCE: All-Russia Scientific Center for Safety Testing of

Biologically Active Substances, Ministry of Public Health of Russian Federation, Kupavna, Russia

SOURCE: Pharmaceutical Chemistry Journal (Translation of

Khimiko-Farmatsevticheskii Zhurnal) (2000),

34(8), 419-423

CODEN: PCJOAU; ISSN: 0091-150X

PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal LANGUAGE: English

AB The purpose of this study was to establish pharmacophores and

antipharmacophores for the antiasthmatic properties and to design mols.

capable of acting simultaneously by several mechanisms.

IT 345218-05-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(computer-aided design of mols. possessing antiasthmatic properties based on computer QSAR anal.)

RN 345218-05-5 CAPLUS

CN Benzamide, 4-[3-hydroxy-2-methyl-5-[[6-(1H-tetrazol-5-yl)hexyl]oxy]phenoxy]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:490074 CAPLUS

DOCUMENT NUMBER: 133:248854

TITLE: Novel tert-Butyl Migration in Copper-Mediated Phenol

Ortho-Oxygenation Implicates a Mechanism Involving Conversion of a 6-Hydroperoxy-2,4-cyclohexadienone

Directly to an o-Quinone

AUTHOR(S): Mandal, Subrata; Macikenas, Dainius; Protasiewicz,

John D.; Sayre, Lawrence M.

CORPORATE SOURCE: Department of Chemistry, Case Western Reserve

University, Cleveland, OH, 44106-7078, USA

SOURCE: Journal of Organic Chemistry (2000), 65(16),

4804-4809

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:248854

Copper mediated ortho-oxygenation of phenolates may proceed through the generation of a 6-peroxy-2,4-cyclohexadienone intermediate. To test this theory, we studied the fate of sodium 4-carbethoxy-2,6-di-tertbutylphenolate, where the ortho-oxygenation sites are blocked by tert-Bu groups. Using the Cu(I) complex of N, N-bis(2-(N-methylbenzimidazol-2yl)ethyl)benzylamine, isolation of the major oxygenated product and characterization by single-crystal X-ray crystallog. and NMR spectroscopy revealed it to be 4-carbethoxy-3,6-di-tert-butyl-1,2-benzoquinone, resulting from a 1,2-migration of a tert-Bu group. The independently prepared 6-hydroperoxide is transformed by the Cu(I)- (or Cu(II)-) ligand complex to the same o-quinone. The observed 1,2-migration of the tert-Bu group appears to reflect an electron demand created by rearrangement of the postulated peroxy intermediate. A mechanism proceeding alternatively through a catechol and subsequent oxidation to the o-quinone seems ruled out by a control study demonstrating that the requisite intermediate to catechol formation would instead eliminate the 2-tert-Bu group.

IT 296252-78-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (novel tert-Bu migration in copper-mediated phenol ortho-oxygenation implicates a mechanism involving conversion of a 6-hydroperoxy-2,4-cyclohexadienone directly to an o-quinone)

RN 296252-78-3 CAPLUS

CN Benzoic acid, 2-[4-(ethoxycarbonyl)phenoxy]-3,4-dihydroxy-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

PUBLISHER:

ACCESSION NUMBER: 2000:216941 CAPLUS

DOCUMENT NUMBER: 132:322237

TITLE: Preparation of poly[(ether)-(ether ether ketone)]

dendrimers by the convergent method

AUTHOR(S): Morikawa, Atsushi; Ono, Katsumichi

CORPORATE SOURCE: Department of Materials Science, Faculty of

Engineering, Ibaraki University, Hitachi, 316-8511,

Japan

SOURCE: Polymer Journal (Tokyo) (2000), 32(3),

255-262

CODEN: POLJB8; ISSN: 0032-3896 Society of Polymer Science, Japan

DOCUMENT TYPE: Journal LANGUAGE: English

New highly branched poly[(ether)-(ether ether ketone)] dendrimers were synthesized by the convergent approach using two building blocks, 3,5-dihydroxybenzyl alc., (I), and 3,5-dihydroxy-4'-(4fluorobenzoyl)diphenyl ether, (II), alternatively. The reaction of p-fluorobenzonitrile and I gave 3,5-bis(4-cyanophenoxy)benzyl alc. (the first generation dendron, G1-OH). After G1-OH was converted to 3,5-bis(4-cyanophenoxy)benzyl bromide (G1-Br), the resultant benzylic bromide functionality was allowed to react with II to yield the second-generation dendron (G2-F). The third-generation dendron (G3-OH) was obtained by the reaction of G2-F and I, and the fourth-generation dendron (G4-F) was obtained by reaction of G3-Br derived from G3-OH, with II. Finally, dendrimers, Den-(G2)3 and Den-(G4)3 were synthesized by reaction of G2-F and G4-F with trifunctional core, resp. Anal. was made of these structurally unambiguous dendrons and dendrimers by gel permeation chromatog. (GPC) and matrix-assisted laser desorption ionization time of flight (MALDI-TOF) mass spectroscopy. 1H and 13C NMR spectra were consistent with the structures of these dendrons and dendrimers.

IT 266370-71-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of poly[(ether)-(ether ether ketone)] dendrimers by convergent
method)

RN 266370-71-2 CAPLUS

CN Methanone, [4-(3,5-dihydroxyphenoxy)phenyl](4-fluorophenyl)- (CA INDEX NAME)

IT 266370-75-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of poly[(ether)-(ether ether ketone)] dendrimers by convergent

method)

RN 266370-75-6 CAPLUS

CN Methanone, [4-(3,5-dihydroxyphenoxy)phenyl](4-fluorophenyl)-, polymer with 5-(hydroxymethyl)-1,3-benzenediol (9CI) (CA INDEX NAME)

CM 1

CRN 266370-71-2 CMF C19 H13 F O4

CM 2

CRN 29654-55-5 CMF C7 H8 O3

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:216938 CAPLUS

DOCUMENT NUMBER: 132:334958

TITLE: Preparation of poly(ether ether ketone) dendrimers by

the divergent method

AUTHOR(S): Morikawa, Atsushi; Ono, Katsumichi

CORPORATE SOURCE: Department of Materials Science, Faculty of

Engineering, Ibaraki University, Hitachi, 316-8511,

Japan

SOURCE: Polymer Journal (Tokyo) (2000), 32(3),

234-242

CODEN: POLJB8; ISSN: 0032-3896

PUBLISHER: Society of Polymer Science, Japan

DOCUMENT TYPE: Journal LANGUAGE: English

AB New highly branched poly(ether ether ketone) dendrimers were synthesized

by the divergent approach through aromatic nucleophilic substitution reactions. 3,5-Dimethoxy-4'-(4-fluorobenzoyl)diphenyl ether, 1, and 1,3,5-tris[p-(3,5-dihydroxyphenoxy)phenyl]benzene, G0-OH, were used as a building block and starting core, resp. The reaction of 1 with ${
m GO-OH}$ gave the first-generation dendrimer (G1-OMe), which possessed 12 methoxy groups on the periphery. After the methoxy groups were converted to hydroxy groups by treatment with pyridine hydrochloride, the resultant phenol functionality (G1-OH) was allowed to react with 1 to yield the second-generation dendrimer (G2-OMe) which possessed 24 methoxy groups. By repeating these procedures G3-OMe dendrimer and G3-OH dendrimer possessing 48 methoxy and hydroxy groups, resp., on the periphery were obtained. 1H and 13C NMR spectra were consistent with the structures of these dendrimers. Mol. wts. and mol. weight distribution determined by gel permeation chromatog. indicated that the dendrimers possessed remarkably narrow mol. weight distribution. Anal. was made of these structurally unambiguous dendrimers by matrix-assisted laser desorption ionization time of flight (MALDI-TOF) mass spectroscopy. The characteristics of these dendrimers, Gn-OMe and Gn-OH, such as solubility and thermal properties were compared.

IT 267421-53-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

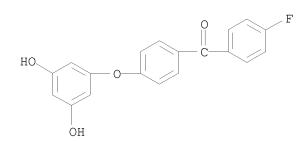
(dendritic; preparation of poly(ether ether ketone) dendrimers by divergent method)

RN 267421-53-4 CAPLUS

CN Methanone, [4-(3,5-dihydroxyphenoxy)phenyl](4-fluorophenyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 266370-71-2 CMF C19 H13 F O4



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:513659 CAPLUS

DOCUMENT NUMBER: 131:257279

TITLE: Synthesis of fluorinated polyphenyl ethers by reaction

of polyfluorinated cyclohexadienones with substituted

phenols

AUTHOR(S): Kovtonyuk, V. N.; Kobrina, L. S.

CORPORATE SOURCE: Novosibirsk Institute of Organic Chemistry, Siberian

Division, Russian Academy of Sciences, Novosibirsk,

630090, Russia

Russian Journal of Organic Chemistry (Translation of SOURCE:

Zhurnal Organicheskoi Khimii) (1999), 35(1),

74-79

CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal LANGUAGE: English

Perfluoro(4-phenoxy-2,5-cyclohexadienone) reacts with sodium 4-nitro- and 4-methoxycarbonylphenoxides in glyme at 65°C to give the corresponding 2,4,6-trifluoro-3,5-bis(aryloxy)-4-[2,4,6-trifluoro-3,5bis(aryloxy)phenoxy]-2,5-cyclohexadienones. Reduction of the latter to phenols, followed by reaction with perfluorotoluene, results in formation of branched polyfluorinated polyphenyl ethers containing NO2 and CO2CH3 functional groups. Reduction of the dinitro polyphenyl ether yields the corresponding diamino derivative A similar reaction sequence gives rise to a linear polyphenyl ether, starting from 6-chloro-2,3,4,5,6-pentafluoro-2,4-

cyclohexadien-1-one and tetrafluororesorcinol.

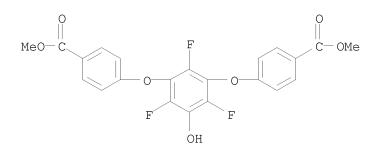
ΙT 245126-30-1P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of fluorinated polyphenyl ethers by reaction of polyfluorinated cyclohexadienones with phenols)

245126-30-1 CAPLUS RN

CN Benzoic acid, 4,4'-[(2,4,6-trifluoro-5-hydroxy-1,3-phenylene)bis(oxy)]bis-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

1999:348617 CAPLUS ACCESSION NUMBER:

131:155777 DOCUMENT NUMBER:

TITLE: Phenolics and flavonoids from Haematoxylon

campechianum

AUTHOR(S): Kandil, F. E.; Michael, H. N.; Ishak, M. S.; Mabry, T.

CORPORATE SOURCE: Chemistry of Tanning Materials and Proteins

Department, National Research Centre, Cairo, Egypt

Phytochemistry (1999), 51(1), 133-134 CODEN: PYTCAS; ISSN: 0031-9422 SOURCE:

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

AB One new natural phenolic, the 5'-O-methyl-7'-Et ester I of p-dehydrodigallic acid, was isolated and identified from the bark of Haematoxylon campechianum. In addition, two known flavonoids, quercetin 3-O-Me ether and genistein and three known phenolics, gallic acid, Me gallate and Et gallate, were also isolated.

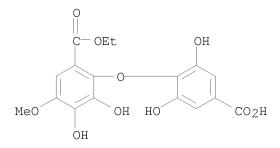
IT 237067-27-5P

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(isolation and structure of phenolics and flavonoids from Haematoxylon campechianum)

RN 237067-27-5 CAPLUS

CN Benzoic acid, 2-(4-carboxy-2,6-dihydroxyphenoxy)-3,4-dihydroxy-5-methoxy-, 1-ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:297219 CAPLUS

DOCUMENT NUMBER: 127:17460

TITLE: A convenient synthesis of 2-alkylated 1,4-benzenediols AUTHOR(S): Ozaki, Yutaka; Hosoya, Ayako; Okamura, Kyouko; Kim,

Sang Won

CORPORATE SOURCE: Faculty Pharmaceutical Sciences, Josai University,

Sakado, 350, Japan

SOURCE: Synlett (1997), (4), 365-366

CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Thieme

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:17460

AB Reaction of 1,4-cyclohexanedione with a variety of aldehydes in the presence of metal halides generated the 2-alkylated 1,4-benzenediols in good yields without any aromatic byproducts.

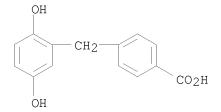
IT 190597-10-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of alkylbenzenediols from cyclohexanedione and aldehydes)

RN 190597-10-5 CAPLUS

CN Benzoic acid, 4-[(2,5-dihydroxyphenyl)methyl]- (CA INDEX NAME)



L4 ANSWER 12 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:680694 CAPLUS

DOCUMENT NUMBER: 126:103762

TITLE: Copper-catalyzed ortho-oxidation of phenols by

dioxygen (tyrosinase mimics) do yields catechols as

primary products

AUTHOR(S): Maumy, M.; Capdevielle, P.

CORPORATE SOURCE: Laboratoire de Chimie Organique de l'ESPCI, associe au

CNRS, 10 rue Vauquelin, Paris, 75231/05, Fr.

SOURCE: Journal of Molecular Catalysis A: Chemical (

1996), 113(1-2), 159-166

CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 126:103762

AB Evidences are provided that catechols [as copper(II)catecholates] are the actual primary products of copper-mediated (catalyzed) ortho-selective oxidation of phenols, on the contrary to a recent claim reporting direct generation of ortho-quinones.

IT 186041-68-9P 186041-70-3P

RL: PNU (Preparation, unclassified); PREP (Preparation) (catechols as primary products from copper-catalyzed ortho-oxidation of

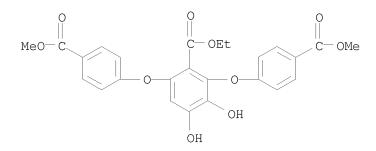
phenols by dioxygen (tyrosinase mimics))

RN 186041-68-9 CAPLUS

CN Benzoic acid, 3,4-dihydroxy-2-[4-(methoxycarbonyl)phenoxy]-, ethyl ester (CA INDEX NAME)

186041-70-3 CAPLUS RN

CN Benzoic acid, 3,4-dihydroxy-2,6-bis[4-(methoxycarbonyl)phenoxy]-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2008 ACS on STN ANSWER 13 OF 21

1996:537861 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 125:275352

TITLE: Galloyl-Derived Orthoquinones as Reactive Partners in Nucleophilic Additions and Diels-Alder Dimerizations:

A Novel Route to the Dehydrodigalloyl Linker Unit of

Agrimoniin-Type Ellagitannins

AUTHOR(S): Feldman, Ken S.; Quideau, Stephane; Appel, Heidi M.

CORPORATE SOURCE: Department of Chemistry, Pennsylvania State University, University Park, PA, 16802, USA Journal of Organic Chemistry (1996), 61(19), SOURCE:

6656-6665

CODEN: JOCEAH; ISSN: 0022-3263

American Chemical Society PUBLISHER:

DOCUMENT TYPE: Journal LANGUAGE: English

CASREACT 125:275352 OTHER SOURCE(S):

GΙ

AB Orthochloranil-mediated oxidation of galloyl mono ethers furnishes the derived orthoquinones in excellent yield. These reactive electrophiles participate in a variety of nucleophilic addition reactions with heteroat. and carbanionic partners. In addition, Lewis acid-mediated dimerization of the orthoquinones provides an efficient route to dehydrodigalloyl-type diaryl ether units, e.g. I, characteristic of several ellagitannin natural products. The implications for ellagitannin biosynthesis and gallotannin-protein covalent attachment are discussed.

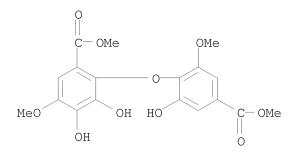
IT 182183-02-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(galloyl-derived orthoquinones as reactive partners in nucleophilic addns. and Diels Alder dimerizations in preparation of dehydrodigalloyl linker unit of agrimoniin-type ellagitannins)

RN 182183-02-4 CAPLUS

CN Benzoic acid, 3,4-dihydroxy-2-[2-hydroxy-6-methoxy-4- (methoxycarbonyl)phenoxy]-5-methoxy-, methyl ester (CA INDEX NAME)



L4 ANSWER 14 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:52555 CAPLUS

DOCUMENT NUMBER: 50:52555

ORIGINAL REFERENCE NO.: 50:10051g-i,10052a-c

TITLE: Synthesis of 3,4-diethoxydiphenyl ether-4',6-

dicarboxylic acid

AUTHOR(S): Tomita, Masao; Kugo, Takehiko

CORPORATE SOURCE: Univ. Kyoto

SOURCE: Yakugaku Zasshi (1955), 75, 1350-4 CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB 4-[6,3,4-HO2C(MeO)2C6H2O]C6H4CO2H (I) (0.5 g.) and 5 ml. AcOH saturated with

HBr at 0° in a sealed tube heated 1 hr. at 105° , cooled, the product washed with water, concentrated in vacuo and the residue extracted with Et20

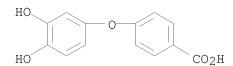
gave 0.25 g. 3,4-di-OH analog (II) of I, columns, m. $196-8^{\circ}$. Methylation of 0.4 g. II in MeOH with CH2N2 in Et2O, removing of the solvent, extracting with Et2O, washing with 3% KOH and saponifying with alc.

KOH

gave I, needles, m. 146-7°. 3,4,6-Me(HO)2C6H2Br (III) (4 g.), m. 92°, in 12 ml. EtOH treated with 1.6 g. NaOH as a 50% aqueous solution and 15 g. Me2SO4 with 6 g. NaOH in 3 portions while heating on a water bath and keeping the reaction alkaline throughout, and the oily layer extracted with Et20, washed with 10% NaOH, and distilled gave 4.2 g. di-Et ether (IV), b6 $140-50^{\circ}$, plates, m. $62-5^{\circ}$. IV (0.5 g.) in 25 ml. azeotropic mixture of C5H5N-H2O treated portionwise with 1.5 g. KMnO4, heated 2 hrs. on a water bath, the product filtered off, the filtrate concentrated in vacuo, and the residue in water acidified with HCl and recrystd. from MeOH gave 6,3,4-Br(EtO)2C6H2CO2H (V), granules, m. 160-2°. Methylation of 11 g. 3,4-(EtO) 2C6H3CO2H by boiling 4 hrs. with 100 ml. MeOH and 10 ml. concentrated H2SO4 gave 12 g. 3,4-(EtO)2C6H3CO2Me (VI), columns, m. 53-4°. VI (11 q.) in 30 ml. AcOH and 9 q. Br in 15 ml. AcOH treated 5 hrs. at 14°, let stand overnight, the product poured into water, extracted with Et20, washed with 2% NaOH, the Et20 removed and the residue recrystd. from MeOH gave 10 g. 6,3,4-Br(EtO)2C6H2CO2Me (VII), needles, m. $55-7^{\circ}$. p-KOC6H4Me (from 1.1 g. p-HOC6H4Me and 0.6 g. KOH), 2.6 g. IV, 0.1 g. Cu, and 0.1 g. (AcO)2Cu heated 4 hrs. at 190-200°, and the product extracted with Et20 and washed with 3% KOH gave 1.2 g. 4-[6,3,4-Me(EtO)2C6H2O]C6H4Me (VIII), b0.2 130-57°. VIII (0.5 g.) and 35 ml. C5H5N-H2O treated with 5 g. KMnO4 portionwise, and the product concentrated extracted with Et20, and dried in vacuo gave 4-[6,3,4-HO2C(EtO)2C6H2O]C6H4CO2H (IX), needles, m. 240-2° (from MeOH); di-Me ester (X), columns, m. 105-7°. p-KOC6H4CO2Me (from 5.5 g. p-HOC6H4CO2Me), 0.5 g. Cu, 0.5 g. (AcO)2Cu, and 10 g. VII heated 5hrs. at $190-200^{\circ}$ and the product treated as in VIII gave 3.4 g. X, m. 106-8°.

RN 859033-56-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



L4 ANSWER 15 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:26059 CAPLUS

DOCUMENT NUMBER: 50:26059

ORIGINAL REFERENCE NO.: 50:5293f-i,5294d

TITLE: Dyes of the anthraquinone series. V.

3-Arylaminoalizarin

AUTHOR(S): Murata, Kazuya; Harada, Kozo; Takiyama, Ken

CORPORATE SOURCE: Hiroshima Univ.

SOURCE: Hiroshima Daigaku Kogakubu Kenkyu Hokoku (1955

), 4, 387-90

CODEN: HIDKAA; ISSN: 0018-2060

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

cf. C.A. 49, 2738d. To 0.5 q. 3-Aminoalizarin and 1 q. bromobenzene in 15 AB g. nitrobenzene, 0.2 g. AcONa and 0.07 g. CuCl2 were added, and the reaction mixture was refluxed for 20 hrs., the solvent distilled off, and the residue was filtered, treated with dilute HCl, and then with dilute alkali to give 28% 3-anilinoalizarin, black-brown powder, m. above 300°, that vat-dyed rayon yellow-orange, and wool dark-purple-red with Cr as mordant, yellow-orange with Sn, and red-purple with Al. Similarly were prepared: 3-(4-nitroanilino)alizarin, m. above 300°, yield 22%, vat-dyed rayon in gray-yellow and wool brown-violet, yellow-orange, and gray-violet with Cr, Sn, and Al, resp.; 3-(2,4-dinitroanilino)alizarin, m. 296°, yield 68%, gave pale-brown rayon and orange-yellow, pale-orange-yellow, and pale-orange-yellow wool; 3-(4carboxyanilino)alizarin, m. 287°, 29%, pale-brown and gray-violet, pale-orange-yellow, and pale-pink; 3-(p-sulfoanilino)alizarin, dyed wool black, yellow-orange, and black-purple; 3-(1-naphthylamino)alizarin, m. above 300°, 39%, pale-yellow-orange and pale-violet-brown, pale-yellow-orange, and dark-red; 3-(2-naphthylamino)alizarin, m. above 300°, 32%, pale-yellow-orange and pale-violet-brown, pale-yellow-orange, and pale-pink; 3-(1-anthraquinonylamino)alizarin, m. 294°, 73%, gray-brown and brown-violet, gray, and gray-purple; 3-(2-anthraquinonylamino)alizarin, m. above 300°, 30%, brown and brown, gray-orange, and brown; 3-(8-amino-1-anthraquinonylamino)alizarin, m. 298°, 67%, brown and pale-orange, -, and pale-brown; 3-(2-methyl-1-anthraquinonylamino)alizarin, m. above 300°, 22%, pale-pink and red-purple, pale-orange-brown, -; 1,8-bis(3alizarylamino) anthraquinone, m. above 300°, 19%, brown and dark-red-purple, pale-orange, and pink; 1,5-bis(3alizarylamino)anthraquinone, m. above 300°, 57%, brown and dark-purple, pale-orange, and pink; 2,6-bis(3-alizarylamino)anthraquinone, m. above 300°, 68%, gray-brown, and gray-brown-violet, pale-yellow-orange, and red-orange; 1,5-bis(3-alizarylamino)-4,8dihydroxyanthraquinone, m. above 300°, 35%, gray-violet and gray-violet, gray-brown, and pale-brown; di-3-alizarylamine, m. above 300°, 35%, gray-brown and gray-black, pale-orange, and brown. ΙT 859032-73-8P, Benzoic acid, p-(3,4-dihydroxy-2-

anthraquinonylamino) -RL: PREP (Preparation) (preparation of)

RN

859032-73-8 CAPLUS INDEX NAME NOT YET ASSIGNED CN

L4 ANSWER 16 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1955:13586 CAPLUS

DOCUMENT NUMBER: 49:13586 ORIGINAL REFERENCE NO.: 49:2684c-f

TITLE: Hyaluronidase-inhibiting substances

INVENTOR(S): Hahn, Ladislaus; Fekete, Janos PATENT ASSIGNEE(S): Aktieselskabet "Ferrosan"

PATENT ASSIGNEE(S): Aktieselskabet "DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

AB Products obtained by condensation of 2,3,4-, 2,3,5-, 2,4,5-, and 2,4,6-trihydroxybenzoic acid with HCHO have a hyaluronidase-inhibiting power > 3000 times greater than salicylic acid and > 30 times greater than previously described inhibitors. Clinical tests indicate value in treatment of rheumatoid arthritis and certain infectious diseases. Thus, 2,4,6-trihydroxybenzoic acid (17 g.) was suspended in 100 g. cold 50% H2SO4 and 4 g. 40% HCHO was added. The reaction mixture was boiled for 5 hrs. with vigorous agitation. The warm product was filtered and the precipitate

pulverized and washed with hot water. The product consisted essentially of polycondensed 2,2',-4,4',6,6'-hexahydroxy-3,3'-dicarboxydiphenylmethane units. The relative hyaluronidase-inhibiting power was <math>3875 (salicylic acid = 1). Polycondensed products consisting of 2,2',3,3',4,4'-hexahydroxy-5,5'-dicarboxydiphenylmethane, <math>2,2',3,3',6,6'-hexahydroxy-4,4'-dicarboxydiphenylmethane, and 2,2',5,5',6,6'-hexahydroxy-3,3'-dicarboxydiphenylmethane units showed relative inhibitory powers of <math>3500, 4000. and 3100-50. Their preparation is described.

IT 857539-72-1, Benzoic acid, 4,4'-methylenebis[2,3,5-trihydroxy-(and polycondensed products)

RN 857539-72-1 CAPLUS

CN Benzoic acid, 4,4'-methylenebis[2,3,5-trihydroxy- (CA INDEX NAME)

L4 ANSWER 17 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1951:52800 CAPLUS

DOCUMENT NUMBER: 45:52800

ORIGINAL REFERENCE NO.: 45:8996h-i,8997a-e

TITLE: The synthesis of certain substituted diaryl sulfones

AUTHOR(S): Ettel, V.; Semonsky, M.; Cerny, A.

CORPORATE SOURCE: United Chem. Met. Works, Prague-Vysocany

SOURCE:

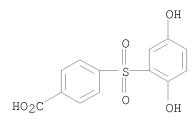
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1950), 15, 653-8
                         CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     The sulfones reported below were without marked antibacterial activity,
     even against Mycobacterium tuberculosis. p-NCC6H4SO2H dissolved (5 g.) in
     20 cc. boiling water was gently heated 10 min. with 32 g. p-quinone (I) in
     10 cc. EtOH, the mixture filtered with charcoal, and the crystals which
     separated in the cold washed with water and recrystd. 3 times from water,
     yielding 2-(p-cyanophenylsulfonyl)hydroquinone (II), colorless needles, m.
     182-3°. II (1.5 g.) dissolved in 10 cc. H2SO4 (d. 1.84), with
     cooling under water, was allowed to stand 5 days at room temperature in the
     open, then poured over ice, the resulting oil crystallized on standing and
     recrystd. from water gave 1.56 g. p-(2,5-dihydroxyphenylsulfonyl)benzamide
     (III), colorless rods, m. 236-7°. III (1.5 g.) refluxed 6 hrs.
     with 30 cc. of 40% H2SO4 and the product which separated on cooling filtered
     off, washed with water, and dried at 45°, yielded 1.5 g.
     p-(2,5-dihydroxyphenylsulfonyl)benzoic acid (IV), colorless, m.
     295-6° (decomposition) (from MeOH). A solution of 5.4 g. II in 20 cc. absolute
     EtOH was saturated with HCl gas at 0°, allowed to stand 48 hrs., and
     the resulting Et p-(2,5-dihydroxyphenylsulfonyl)benzimidate-HCl (V) washed
     with 5 cc. EtOH, then 10 cc. dry Et2O, and kept over concentrated H2SO4;
precipitation
     of the filtrate with Et2O gave addnl. V (total yield, 6.1 g.), colorless,
     m. 152-3^{\circ}. V (2.5 g.) suspended in 10 cc. cold EtOH was allowed to
     stand 3.5 hrs. in 5 cc. of absolute alc. NH3 (7.5%) at room temperature, and
the
     crude p-(2,5-dihydroxyphenylsulfonyl)benzamidine (VI) filtered off at the
     pump, washed with water, then EtOH, and dried in vacuo over KOH; addnl.
     VI, separated from the filtrate overnight. VI repeatedly crystallized from
EtOH
     with alc. NH3, formed yellow microcrystals, m. 241-2°; picrate
     (prepared from V), m. 242-4^{\circ} (decomposition) (from aqueous EtOH).
     p-NCC6H4SO2H (10 g.) dissolved in 45 cc. boiling water was gently heated
     10 min. with 9.8 g. thymoquinone (VII) in 60 cc. EtOH, and filtered with
     charcoal; the oil which separated, crystallized in the cold, yielding 17 q.
     3-(?)-(p-cyanophenylsulfonyl)thymohydroquinone (VIII), faintly yellowish,
     m. 152-3° (from aqueous EtOH). Crude 4,3-HO(HO2C)C6H3SO2C1 (from 56 q.
     of the SO3H acid) was shaken with 252 g. NaHSO3 in 500 cc. water (the
     solution being kept alkaline by slow addition of 50% NaOH during reaction), the
     cooled filtrate acidified with 60% H2SO4, and the 5-sulfinosalicylic acid
     (IX) filtered off and dried at 40^{\circ}; yield, 35-7 g., m.
     202-5° (decomposition, sealed tube). IX (10 g.) in 40 cc. of 10% H2SO4
     stirred constantly at 70° with 4.8 g. I in 50 cc. water, and the
     solution cooled, gave white crystals of 2-(4-hydroxy-3-
     carboxyphenylsulfonyl) hydroquinone (X); repeated recrystn. from aqueous EtOH
     yielded X.H2O, m. 234-7° (decomposition). A IX (4 g.) in 30 cc. of 50%
     aqueous EtOH slowly added at 70° to 3 g. VII in 10 cc. of EtOH gave a
     brick-red oil; the cold solution was diluted with water, and the oil separated
and
     kept in a desiccator over silica gel until it was triturated with CHCl3,
     giving 3-(?)-(4-hydroxy-3-carboxyphenylsulfonyl)thymohydroquinone (XI),
     colorless, m. 179-80^{\circ} (from xylene). The solubilities of the above
     compds. are reported in general terms for various organic solvents.
ΙT
     859033-53-7P, Benzoic acid, p-(2,5-dihydroxyphenylsulfonyl)-
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Collection of Czechoslovak Chemical Communications (

860683-03-0P, Benzamide, p-(2,5-dihydroxyphenylsulfonyl)-RL: PREP (Preparation)

(preparation of) 859033-53-7 CAPLUS RN

CN INDEX NAME NOT YET ASSIGNED



RN 860683-03-0 CAPLUS

CN Benzamide, 4-[(2,5-dihydroxyphenyl)sulfonyl]- (CA INDEX NAME)

ANSWER 18 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1951:41344 CAPLUS

DOCUMENT NUMBER: 45:41344

ORIGINAL REFERENCE NO.: 45:7048e-i,7049a-i

TITLE: Aromatic keto- and hydroxy-polyethers as lignin

models. III

AUTHOR(S): Leopold, Bengt CORPORATE SOURCE: Kgl. Tek. Hogskolan, Stockholm

SOURCE:

Acta Chemica Scandinavica (1950), 4, 1523-37

CODEN: ACHSE7; ISSN: 0904-213X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 45:41344 For diagram(s), see printed CA Issue. GΙ

cf. C.A. 44, 7338g. A series of lignin models of type (I) were AΒ synthesized and oxidized with PhNO2 and alkali; oxidation was preceded by alkaline fission of the ether linkages. In all expts. 0.5-2 q. substance was heated 2 hrs. at 180° with 60 cc. of 2 N NaOH and 8 cc. PhNO2/g. substance. The yields of vanillin (II), vanillic acid (III), 5-formylvanillin (IV), and 2,3,5-HO(MeO)(OHC)C6H2CO2H (V) in Series A (I, R' = CH:CHMe), from (VI) (R = H, n = 0), (VII) (R = H, n = 1), (VIII) (R = H) Me, n = 0), and (IX) (R = Me, n = 1) were 69, 6, 1, and 11; 66, 8, trace, and 9; 0, 0, -, and -; and 70, 3, 2, and 12%, resp. The yield of II in Series B (I, R' = Pr) from (X) (R = H, n = 0), (XI) (R = H, n = 1), (XII)

(R = Me, n = 1), and (XIII) (R = Me, n = 2) was 60, 67, 67, and 62%, resp., and of III 6, -, 5, and -, resp. In series C, compds. of type 4,3-HO(MeO)C6H3R (XIV) were oxidized. The yield of II for R = CH2OH, CH2SO3(Ba/2), CH:CH2, Ac, COCH2OH, Pr, COEt, COCH(OH)Me, CH2CH:CH2, CH:CHMe, and CH:CHCHO in XIV was 82+, 80, 80, 81, 66, 17, 30, 33, 88, 90, and 86%, resp., and the yield of III was 3, -, 6, 4, 10, -, -, 21, -, trace, and 4%, resp. In Series D, compds. of type 5,4,3-R'(HO)(MeO)C5H2R (XV) were oxidized. The yields of II, IV, and V from (XVI) (XV, R = R' = CH2OH), (XVII) (R = CH2CH:CH2, R' = CH2OH), (XVIII) (R = CH0, R' = CH2OH)CH2CH:CH2), and IV (R = R' = CHO) were 0.8, 13, and 6; 2.2, 9, and 11; 1.6, 20, and 6; and 1.5, 12, and 26% resp. In series E, compds. of type (XIX) were oxidized. The yield of II from XIX (R = H, n = 2, 3, and 4)and XIX (R = Me, n = 2, 3, and 4) was 63, 60, 60, 88, 71, and 73% resp., and the yield of III was 11, 12, -, 0, 4, and -%, resp. In Series F, compds. of type (XX) were oxidized. The yield of II from XX (X = OH, n =2, 3, 4) and XX (X = SO3(Ba/2), n = 2, 3, and 4) was 87, 74, 72, 83, 70, and 71%, resp. Some members of series E (XIX, R = Me, n = 2 and 3) and Series F (XX, X = OH, n = 2 and 3) were heated 2 hrs. at 180° with 60 cc. 2 N NaOH to yield 14, 18, 3, and trace %, resp., of veratric acid and 75% acetoguaiacone (XXI), 75% XXI (and 12% III), 18% vinyl guaiacol (XXII), and 23% XXII, resp. In the preparation of dehydrodiisoeugenol (VI), to 50 g. freshly distilled isoeugenol in 450 cc. 95% EtOH and 200 cc. H2O, were added 70 g. FeCl3 in 200 cc. H2O and a few crystals VI, the mixture cooled, and the precipitate of VI separated, washed with 45% EtOH, and recrystd. from EtOH;

the yield of VI was 15 g., m. 132-3°. In the preparation of (acetoguaiacyl)dehydrodiisoeugenol Me ether (IX), 5 g. $\alpha\text{-bromoacetoveratrone}$ (XXIII), 6.3 g. VI, and 10 g. anhydrous K2CO3 in 100 cc. absolute MeCOEt were refluxed 30 min., the mixture washed with ${\tt H2O}$, and the MeCOEt layer dried over anhydrous Na2SO4 and concentrated in vacuo to yield 7.95 g. IX, m. 123-4° (from EtOH). (Acetoguaiacyl)dehydrodiisoeuge nol benzoate (XXIV) was prepared by treating 4.2 g. 3,4-MeO(BzO)C6H3COCH2Br (XXV), 4 g. VI, and 10 g. K2CO3 in 100 cc. MeCOEt as above; the yield of XXIV was $3.7 \text{ g., m. } 124-5^{\circ} \text{ (from EtOH).} \text{ XXIV } (2.7 \text{ g.) refluxed}$ with 2 cc. piperidine (XXVI) in 75 cc. EtOH 30 min., and the mixture poured into H2O, acidified, and treated with EtOH, yielded 1.6 q. crystals which were dissolved in CHCl3, the solution filtered through Al2O3, and the CHCl3 evaporated to yield (acetoguaiacyl)dehydrodiisoeugenol (VII), m. 129-30° (from dilute EtOH). Acetoguaiacyldihydrodehydrodiisoeugenol Me ether (XII), m. $99-100^{\circ}$, was prepared in 78% yield from XXIII and X as described above for IX; di(acetoguaiacyl)dihydrodehydrodiisoeugenol Me ether (XIII) (I, R' = Pr, R = Me, n = 2), m. $114-15^{\circ}$, in 79% yield from ω -bromoacetoguaiacylacetoguaiacone Me ether and X. XI benzoate, m. $98-9^{\circ}$, in 54% yield from XXV and X, and XI, m. 82-3°, in 73% yield by the debenzoylation of XI benzoate with XXVI. Methylation of XI with CH2N2 in Et2O gave XII, m. 100-101°. Dihydro-3-methoxy-4-benzyloxyphenacyl coerulignol ether (XXVII) was prepared as follows: To 10 q. XXI and 15 cc. PhCH2Cl in 150 cc. EtOH was added 3.7 g. NaOH, the mixture refluxed 1.5 hrs., poured into H2O, extracted with Et2O, and the Et20 solution washed with H2O, dried over anhydrous Na2SO4, and evaporated

to yield an oil from which was separated 13.3 g. acetoguaiacone benzyl ether, 4,2-Ac(MeO)C6H3OCH2Ph (XXVIII), m. 86-6.5° (from petr. ether). To 10 g. XXVIII in 100 cc. CHCl3 was added 6.25 g. Br in 50 cc. CHCl3, and the mixture washed with NaHCO3 solution and H2O, dried over anhydrous Na2SO4 and

evaporated to yield 9.7 g. ω -bromoacetoguaiacone benzyl ether (XXIX), m. 102.5-103° (from C6H6-petr. ether). XXIX (5 g.) and 2.55 g. coerulignol, treated as described for the preparation of IX, yielded 5.5 g. 3-methoxy-4-(benzyloxy)phenacyl coerulignol ether, m. 86.5-7.5° (from Et2O), 4 g. of which with 4 g. (Me2CHO)3Al in 30 cc. absolute iso-PrOH yielded 3.5 g. XXVII, m. 55-7°, which in vacuo at 70° lost 1 mole H2O to give anhydrous XXVII, m. 62-3°. The oxidation products were steam-distilled to remove nitrogenous compds., acidified, extracted continuously for 24 hrs. with C6H6, and the C6H6 exts. shaken with bisulfite, bicarbonate, and NaOH. A detailed description is given for the separation and identification of the oxidation reaction products. In general it was found that units connected only by ether linkages gave high yields of II and III, and units connected by C-C linkages gave no II or III. 857560-43-1P, Acetophenone, 2''-(4-acetyl-2-methoxyphenoxy)-4'-(4-

IT 857560-43-1P, Acetophenone, 2''-(4-acetyl-2-methoxyphenoxy)-4'-(4-hydroxy-2-methoxyphenacyloxy)-2,4'''-oxybis[3'-methoxy-

RN 857560-43-1 CAPLUS

CN Ethanone, 2-[4-[2-(4-acetyl-2-methoxyphenoxy)acetyl]-2-methoxyphenoxy]-1[2-(4-acetyl-2-methoxyphenoxy)-4-hydroxy-6-methoxyphenyl]- (CA INDEX NAME)

L4 ANSWER 19 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1949:41364 CAPLUS

DOCUMENT NUMBER: 43:41364

ORIGINAL REFERENCE NO.: 43:7449q-i,7450a-f

TITLE: Compounds related to 4,4'-diaminodiphenyl sulfone.

p-Arylsulfonylphenylethylamines and related compounds

AUTHOR(S): Burton, H.; Hu, P. F.

SOURCE: Journal of the Chemical Society (1949)

178-81

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB cf. C.A. 42, 6356ag. 4-02NC6H4S02C6H4Me-4 with Cr03 in AcOH-Ac20-H2S04 gives 4-(p-nitrophenylsulfonyl)benzylidene diacetate, m. 150-1°; hydrolysis gives 74% 4-(p-nitrophenylsulfonyl)benzaldehyde, m. 214-15°. 2,5-(H0)2C6H3S02C6H4CN-4 with the Stephen reagent from 9 g. anhydrous SnCl2 in 130 cc. ether (shaken 7 hrs.) gives 5 g. 4-(2,5-dihydroxyphenylsulfonyl)benzaldehyde, m. 200-1°. p-MeO3SC6H4CHO (6 g.), 7 g. hippuric acid, 8 g. AcONa, and 30 cc. Ac20, heated 1 hr. on the steam bath, give 5 g. 5-keto-2-phenyl-4-(p-

ΙT

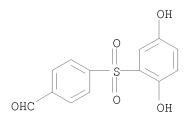
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methylsulfonylbenzylidene)-4,5-dihydrooxazole (I), yellow, m.
     186-7°; hydrolysis of I with warm dilute NaOH gives
     \alpha-benzamido-p-(methylsulfonyl).-cinnamic acid (II), m. 245-6°
     (decomposition). Analogs of I: 4-(p-Phenylsulfonyl), yellow, m. 222-3°,
     73%; 4-(4-p-chlorophenylsulfonyl), orange-red, m. 212-13°, 60%;
     4-(4-p-methoxyphenylsulfonyl), yellow, m. 195-6°, 90%;
     4-(p-N-acetylsulfamyl) analog (III), orange-red, m. 240-1^{\circ}
     (decomposition), 62%. p-PhSO2 analog of II, m. 226-7°. I (9 g.),
     reduced with 5.6 g. red P and 35 cc. HI in 35 cc. Ac2O, gives 5.5 g.
     (p-RSO2C6H4)CH2CH (NH2) CO2H, where R is Me, m. 270° (decomposition).
     The following were similarly prepared (R given): Ph, m. 252°
     (decomposition), 70%; p-chlorophenyl, m. 259° (decomposition), 73%;
     p-hydroxyphenyl, with 1 mol. H2O, m. 265° (decomposition), 62% from the
     MeO compound; p-aminophenyl (IIIA), yellow, m. 195° (decomposition), 40%.
     III (5 g.) in 60 cc. EtOH at 75^{\circ}, treated with 26 g. 3% Na-Hg and,
     after 1.5 hrs., with an addnl. 26 g., with stirring for an addnl. 2.5
     hrs., and the residue in 15 cc. H2O acidified with concentrated HCl, gives
     \alpha\text{-benzamido-}\beta\text{-}(\text{p-sulfamylphenyl})\,\text{alanine-HCl, m.}~237^{\circ}
     (decomposition). The acids could not be decarboxylated by heating alone in
     vacuo or in C3H5(OH)3, Ph2NH, or paraffin. The appropriate aldehyde,
     heated at 100° with CH2(CO2H)2 in C5H5N containing a little piperidine
     until effervescence ceases and then treated with an excess 6 N HCl, gives
     67-87% of the p-(R-sulfonyl)cinnamic acids, p-RSO2C6H4CH:CHCO2H (R
     given):Ph, m. 298°; p-chlorophenyl, m. 282°;
     p-methoxyphenyl, m. 259-61° (decomposition); p-nitrophenyl (IV), m. 273-5°; amino (V), m. 276° (decomposition). The Na salts in H2O
     were reduced over Raney Ni at room temperature and atmospheric pressure,
giving 77-90%
     of the \beta-[p-(R-sulfonyl)phenyl] propionic acids: R = Ph, m.
     194-5°; p-methoxyphenyl, m. 168°; 2,5-dihydroxyphenyl, m.
     180°. Catalytic reduction of IV gives the p-aminophenyl analog
     [HCl salt, m. 209^{\circ} (decomposition); Ac derivative, with 1 mol. H2O, m.
     215°]. Reduction of IV with Fe powder in aqueous EtOH containing HCl gives
     p-(4-aminophenylsulfonyl)cinnamic acid, whose Ac derivative m. 237°.
     Reduction of 3 g. V with 3% Na-Hg in dilute NaOH gives 2.5 g.
     \beta-(p-sulfamylphenyl)propionic acid (VI), m. 148-50°. The
     2-[p-(R-sulfonyl)phenyl]ethylamine-HCl were prepared in 40-60% yields from
     the propionic acids through the acid chlorides and azides (R given): Ph,
     m. 184-5°; p-chlorophenyl, m. 251°; p-methoxyphenyl, m.
     170°; 2,5-dihydroxyphenyl, m. 197°; p-aminophenyl (free
     base), m. 129°; amino (VII), m. 149°. 1-[p-(R-
     sulfonyl)phenyl]ethylamines were prepared in 50-66% yields from the reaction
     of the appropriate ketone and 4 mols. HCO2NH4 and hydrolysis of the insol.
     material with boiling concentrated HCl: Ph, m., 85° (HCl salt, m.
     218-19°); amino, m. 172°. p-Methylsulfonyldiphenylamine, Ph(MeSO2C6H4)CHNH2 (VIII), m. 92-3°; p-PhSO2 analog, m.
     154-5°, 80%. p-H2NC6H4Ac gives 20% 4,4'-diacetyldiphenyl disulfide, m. 92-3°; 2.4 g. yields 1 g. p-sulfamylacetophenone, m.
     178-9°. p-AcC6H4N2Cl and Na2S give 4,4'-diacetyldiphenyl sulfide,
     m. 88°, which yields 4,4'-diacetyldiphenyl sulfone, m. 209°.
     VI-VIII had little or no activity against Streptococcus hemolyticus at a
     dilution of 1:1000. IIIa is also inactive.
     858215-86-8P, Hydrocinnamic acid, p-(2,5-dihydroxyphenylsulfonyl)-
     860679-98-7P, Benzaldehyde, p-(2,5-dihydroxyphenylsulfonyl)-
     RL: PREP (Preparation)
        (preparation of)
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RN 858215-86-8 CAPLUS

CN Benzenepropanoic acid, 4-[(2,5-dihydroxyphenyl)sulfonyl]- (CA INDEX NAME)

RN 860679-98-7 CAPLUS

CN Benzaldehyde, 4-[(2,5-dihydroxyphenyl)sulfonyl]- (CA INDEX NAME)



L4 ANSWER 20 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1928:13476 CAPLUS

DOCUMENT NUMBER: 22:13476

ORIGINAL REFERENCE NO.: 22:1583h-i,1584a-e

TITLE: Reactions of diazomethane on ethyl

phloroglucinoldicarboxylate and its derivatives and

their reaction with nitric acid

AUTHOR(S): Leuchs, Hermann

SOURCE: Justus Liebigs Annalen der Chemie (1928),

460, 1-32

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB (With Ilse Waldorf). The ester, C12H14O7 (3.87 g.), 0.25 g. FeCl3 and 3 g. BzCl in 50 cc. ligroin, boiled 1 hr., give 0.6-1.2 g. Et O-benzoylphloroglucinoldicarboxylate (I), m. 137-8°; FeCl3 gives a red color; an oxime could not be prepared; with AcCl it gives the tri-Ac derivative, m. 96-8°. I (1.25 g.) and 0.5 g. CH2N2 in Et2O, allowed to stand 1 hr. between 0° and 20°, give 0.4-0.6 g. of the O-di-Me ether (II) m. 106°, and 0.8-0.6 g. of the O-mono-Me ether, m. 116-8°. II is saponified by EtOH-NaOH, giving Et O-dimethylphloroglucinoldicarboxylate (III) m. 146-7°; the free acid, m. 186-8° (decomposition); BrHBr in AcOH gives the compound C9H9O5Br, m. 220° (decomposition). III is also obtained by the methylation of the ester at 15° (2.2 mols. CH2N2); 1.2 mols. CH2N2 give 40% of the mono-Me ether, m. 107.5-8.5°. O-Trimethylphloroglucinoldicarboxylic acid (IV), decomps. 260°, is

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obtained by saponification of the ester by EtOH-NaOH; with Br it gives
dibromophloroglucinol tri-Me ether, m. 129-30°. The Br derivative of
IV, m. 165-73^{\circ} (decomposition) is obtained by saponification of the ester, m.
51°. The nitro derivative of IV, m. 132-5°, decomps.
180°, is likewise obtained by saponification of the ester, b15 about
250^{\circ}; with CH2N2 the acid gives the di-Me ether, m. 70-1^{\circ}.
Nitrophloroglucinol tri-Me ether, m. 151-2°. Et
1,2,3,5-tetramethoxybenzenedicarboxylate, from the phenol and CH2N2, m.
64-5°. Et N-dimethylaminophloroglucinoldicarboxylic acid, m.
151-2°; FeCl3 gives a red color. Et O-
trimethylphloracetophenonedicarboxylate, from the phenol ester and CH2N2,
oily; the free acid, m. 142-4°, decomps. 170°; CH2N2 and the
acid give the di-Me ester, m. 74°. (With Paul Sander.) The action
of HNO3 (d. 1.39) on the ester C12H1407 at 10-25^{\circ} gives 46-56\% of
tetra-Et phlorazurintetracarboxylate (V), C24H23O14N (formerly considered
a ketenequinone, C22H21O13N, C. A. 3, 542), m. 162-3°; CH2N2 gives
a dark red tri-Me ether, m. 100-1°; heating V in AcOEt or C6H6
gives 55-62% of the compound C22H19O13N (VI), light reddish brown, m.
230-2^{\circ}. V and CH23N2 give the dark red compound, C26H27O13N, m. 109-10^{\circ}, reduced by Zn dust in AcOH to the yellow compound,
C24H29O13N, m. 136°. Reduction of VI with Zn and AcOH gives the compound C22H21O13N, yellow, m. 198-212°; CH2N2 gives the compound, C27H31O13N, m. 120-1°. (With W. Robert Leuchs.) Reduction of VI
gives tetra-Et trihydroxyphenoxazone-1,3,6,8-tetracarboxylate, brick-red,
m. 192-3°, whose tri-Ac derivative m. 172-4°. CH2N2 gives the
O-tri-Me derivative, light yellow-red, m. 112-3°, reduced by Zn in AcOH
to the tri-Me derivative of the oxazine, C27H31O13N, pale yellow, m.
119.5-20.5°. EtOH-NH2OH gives a red oxime, C12H14O7N2 (VII), m.
138°, and a yellow oxime, C12H13O13N (VIII), m. 141°. HNO3
oxidizes VII to Et nitrophloroglucinoldicarboxylate. Reduction of VII
with Zn in AcOH gives the diamine, C12H16O6N2, m. 126-7°; CH2N2
gives the compound C13 H1406N2, m. 130-2^{\circ}. VIII gives the same
oxidation product as VII; CH2N2 gives the compound C14H15O7N, m.
162-3°. Tetra-Et tetrahydroxyphenoxazine-1,3,6,8-tetracarboxylate,
golden yellow, m. 195-7°; it crysts. with 14% AcOH, m.
185-7°; O-tetra-Me derivative, light yellow, m. 98-9°.
yellow acid, C24H23O14N (C. A. 3, 542) (IX) is obtained from the ester
C12H1407 with HNO3 (d. 1.45) in 40-50% yields, together with 30-40% of the
nitro ester, C12H1308N; IX decomps. at 216°; the di-Ac derivative, m.
185-7^{\circ} (Me ester, m. 140-2^{\circ}). IX yields a tri-Me derivative, m.
96-8^{\circ}. Reduction of IX gives the compound C24H25O14N, m.
145-7°. IX and NH2OH in EtOH-KOH give the compound C21H21O12N3,
sinters 187°, decomps. 207° (HNO3 gives the compound
C21H20012N2, m. 153-4^{\circ}), and the monoxime, C23H24012N2, m.
130-1^{\circ} (di-Me ether, m. 67-8°). Tetra-Et
sym-hexahydroxydiphenylaminetetracarboxylate, C24H27O14N, m.
186-7^{\circ}; Ac derivative, m. 207-8^{\circ}; a by-product is the greenish
yellow compound C24H25O13N, m. 187° (tetra-Ac derivative, m.
204-5°; di-Me ether, yellow, m. 124-5°; tri-Me ether,
yellow, m. 84-6^{\circ}).
857806-18-9, Isophthalic acid, 4,4'-iminobis[2,5,6-trihydroxy-
   (derivs.)
857806-18-9 CAPLUS
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Isophthalic acid, 4,4'-iminobis[2,5,6-trihydroxy- (3CI) (CA INDEX NAME)

L4 ANSWER 21 OF 21 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1909:250 CAPLUS

DOCUMENT NUMBER: 3:250

ORIGINAL REFERENCE NO.: 3:55i,56a-h

TITLE: Carbomethoxy Derivatives of Phenolcarboxylic Acids and

their Employment for Syntheses

AUTHOR(S): Fischer, Emil

CORPORATE SOURCE: Chem. Inst., Univ. Berlin

SOURCE: Berichte der Deutschen Chemischen Gesellschaft (

1909), 41, 2875-91

CODEN: BDCGAS; ISSN: 0365-9496

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

p-Carbomethoxyhydroxybenzoic acid, MeO2COC6H4CO2H, from p-hydroxybenzoic acid and methyl chlorcarbonate, in presence of 1N aqueous NaOH (cf. preceding abstract). Slender, colorless needles, m. 179° (corrected) previously softening. Yield quantitative. It gives no color with FeCl3 or Millon's reagent and is hydrolyzed immediately to the hydroxybenzoic acid by solution in cold aqueous NaOH. Chloride, from the acid and PC15; long, colorless, radial needles, m. 82-3° (corrected) previously softening. It boils without decomposition (10-15 min.) and is relatively stable in air. Yield, 90%. Ethyl glycollate converts it into ethyl p-carbomethoxyhydroxy-benzoylglycinate, MeO2COC6H4CONHCH2CO2Et; colorless, lustrous plates, m. 63°, previously softening. Yield, practically quantitative. With alkali it gives p-hydroxyhippuric acid, HOC6H4CONHCH2CO2H, m. and decomposes 238° (240° corrected). Schotten gives m. 228°; his material was from the urine of dogs fed on p-hydroxy-benzoic acid and from that of men fed on Na hydro-p-cumarate. The acid may also be obtained from the chloride and glycocoll, in alkaline solution, but the yield is only 50 instead of 93%. The compounds described below were prepared in a similar manner to the preceding ones. Dicarbomethoxyprotocatechuic acid, (MeO2CO) 2C6H3CO2H; colorless, slender needles, m. 165-6° (corrected), previously softening. Yield, 90%. Chloride, colorless needles, softens about 116°, m. 118° (corrected). Yield, 90-5%. Tri-carbomethoxygallic acid, (MeO2CO)3C6H2CO2H, was prepared in an atmosphere of H. Bundles of colorless, thin prisms, softens about 130°, m. 136-41° (corrected). Yield, 80-5%. Brom derivative, crystalline. Pyridine salt. In presence of excess of the base, the acid is hydrolyzed. Tricarbethoxygallic acid, colorless, lustrous plates, m. 96-7° (corrected), previously softening. Yield, almost quantitative. The carbomethoxy acid is hydrolyzed completely by heating with cold HCl (20%), or by the action of cold aqueous NaOH or NH3; with 2NaOH, at 20°, dicarbomethoxygallic acid is formed, colorless crystals resembling biconvex lenses, m. 160° (corrected), previously softening. Yield, 90%. It is probable that the OH is in the p-position.

Tricarbomethoxygalloyl chloride, long needles, m. 86° (corrected), previously softening. Yield, 94%. It gives colorless compounds with NH3 and PhNMe2. Anilide, (MeO2CO) 3C6H2CONHPh bundles of pointed needles, m. 175-6°, previously softening. Tricarbomethoxygalloyl-phydroxybenzoic acid, (MeO2CO)3C6H2COOC6H4CO2H, from the chloride, p-hydroxybenzoic acid and aqueous NaOH. Bundles of thin prisms, m. 165° (corrected), previously softening Aqueous NH3 hydrolyzes it to galloyl-p-hydroxybenzoic acid, (HO)3C6H2COOC6H4CO2H heavy, sandy lustrous, crystalline powder consisting of microscopic, acute angled plates, m., blackens and evolves gas about 260° (corrected). Yield, 60%. Its alkali solution quickly becomes brown in air and its color reactions with FeC13 and KNC resemble those of gallic acid. Alkalies hydrolyze it to its constituent acids. Tricarbomethoxy-galloyl chloride and dicarbomethoxygallic acid, in presence of NaOH, yield an amorphous compound, which, by the action of aqueous NH3, forms what is probably di-gallic acid. Thin, short, microscopic prisms, or needles, m., darkens and evolves gas about $275-80^{\circ}$. The applications of this method of synthesis are very numerous. Hitherto it had not been possible to prepare chlorides of phenolcarboxylic acids, because the PC15 attacked both the CO2H and OH. The interaction of salicylic acid and methyl chlorcarbonate is attended with considerable difficulties, but methyl salicylate combines easily.

RN 861603-50-1 CAPLUS

CN Benzoic acid, 4-[(3,4,5-trihydroxyphenyl)methyl]- (CA INDEX NAME)